

Toluene  
108-88-3 | DTXSID7021360

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $9.74 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $2.74 \times 10^{-1}$

**Confidence level:**  $9.04 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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1,3,5-Cycloheptatriene

**Measured:**  $9.69 \times 10^{-11}$

**Predicted:**  $1.00 \times 10^{-10}$

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Cyclohepta-1,3-diene

**Measured:**  $1.39 \times 10^{-10}$

**Predicted:**  $1.35 \times 10^{-10}$

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1,4-Cyclohexadiene

**Measured:**  $1.00 \times 10^{-10}$

**Predicted:**  $1.11 \times 10^{-10}$

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(E)-Crotonaldehyde

**Measured:**  $3.61 \times 10^{-11}$

**Predicted:**  $3.73 \times 10^{-11}$

Image not found

Crotonaldehyde

**Measured:**  $3.61 \times 10^{-11}$

**Predicted:**  $3.73 \times 10^{-11}$